Supplementary Material for

Investigating Intergenerational Differences in Human PCB Exposure due to Variable Emissions and Reproductive Characteristics.

Cristina Leslie Quinn[1], Frank Wania[1*], Gertje Czub[2], Knut Breivik[3,4]

[1] Department of Chemistry and Department of Physical and Environmental Sciences, University of Toronto Scarborough, Scarborough, Ontario, Canada

[2] Swedish Chemicals Agency, Sundbyberg, Sweden

[3] Norwegian Institute for Air Research, Kjeller, Norway

[4] University of Oslo, Department of Chemistry, Oslo, Norway

Corresponding author:

Phone: 416-287-7225

Fax: 416-287-7279

Email: frank.wania@utoronto.ca

Table of Contents for Supplementary Materials

1. Exposure Calculations

Exposure was defined similar to the method by von Goetz et al. (2010). Postnatal exposure, E_{post}, was calculated by summation of the lipid normalized concentrations of the infant at 5 day intervals over the six month period of lactational transfer as follows:

$$E_{post} = \sum_{t=0}^{t=0.5} C_B \cdot 1.3799 \times 10^{-2}$$

where C_B is the concentration of PCB-153 (ng/g lipid) at a given time, t (years), and 1.38×10^{-2} is the conversion factor for the number of years per 5 day interval. E_{post} is represented in Figure 1 by the area shaded in dark grey. The cumulative lifetime exposure was calculated by summation of the lipid normalized concentration over the 79 year lifetime by:

$$E_{life} = \sum_{t=0}^{t=1} C_B \cdot 1.38 \times 10^{-2} + \sum_{t=1}^{t=79} C_B$$

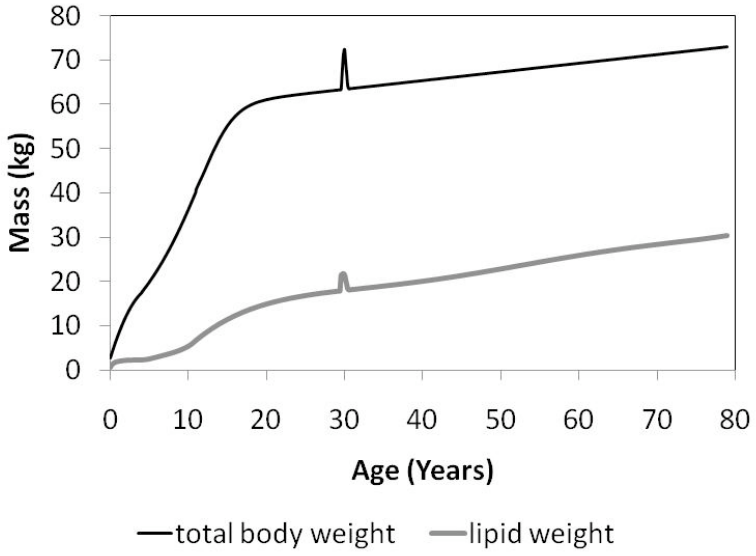
E_{life} is represented in Figure 1 by the addition of the dark grey and light grey shaded area.

2. Dietary Parameters

The dietary composition for time-variant conditions mimics that of the Swedish population for 25-year old individuals (Czub and McLachlan 2004). For the steady-state calculations, the dietary composition was constant over the individual's lifetime. To represent a "worst case scenario", food consumption was set equal to the maximum values that occured between 1930 and 2005. For a female, this corresponds to 49.87 g lipid per day of dairy products, 11.58 g lipid per day of beef, and 75.57 g wet weight per day of fish.

3. Growth Curve

The growth curve for the default woman is illustrated in Supplementary Material Figure 1 below and was calculated according to (Moser and McLachlan 2002). The default female is defined as the primiparous woman who gives birth at the age of 30 and breastfeeds the infant for 6 months.

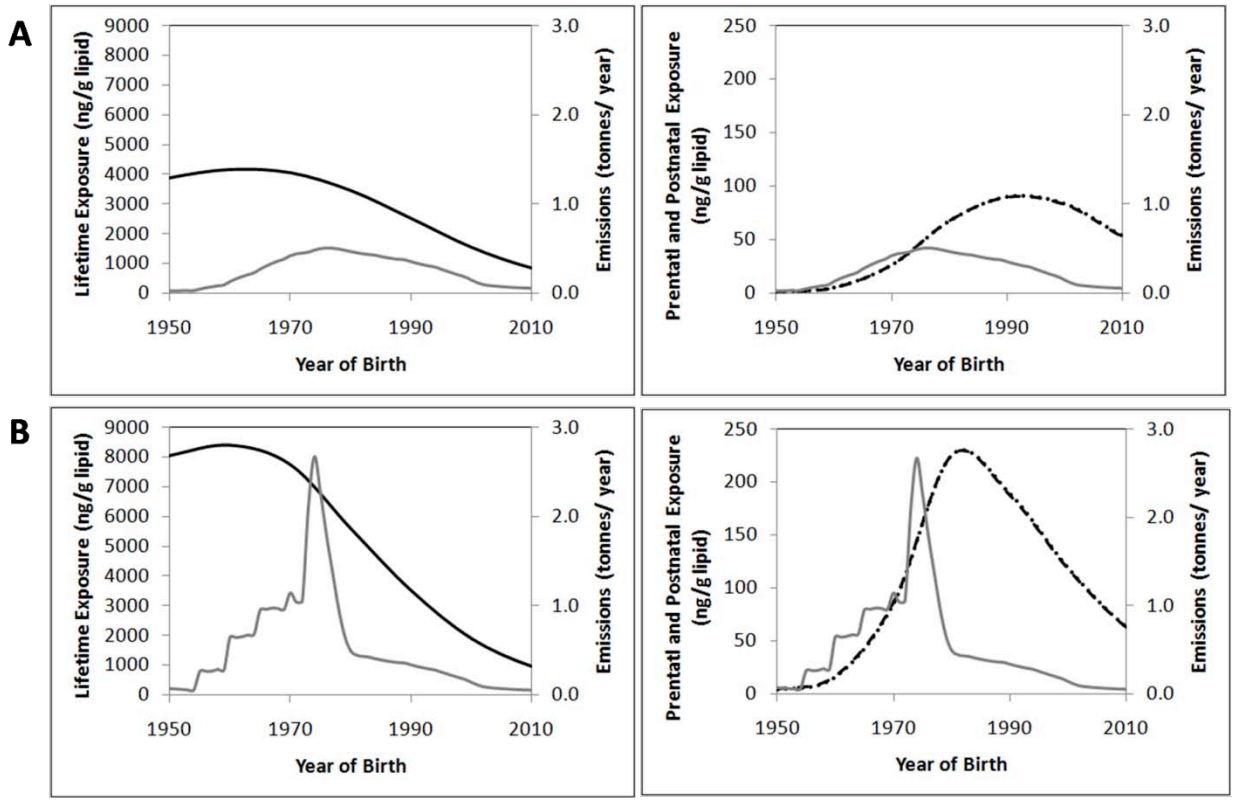


Supplemental Material, Figure 1: Growth curve for the default female.

4. Emissions Scenarios

Previous studies identified that the uncertainty in emission time trends may have led to the underestimation of emission inventories (Breivik et al. 2010). For this reason, three emission scenarios were used to predict PCB exposure in the Swedish Baltic region (See Supplementary Material, Figure 2) (Breivik et al. 2010). Scenario 1 represents the recommended maximum historical atmospheric emissions inventory for the region (Breivik et al. 2007). Unfortunately, this scenario lacks empirical emissions data from the early stages of PCB production (Breivik et al. 2002). As an alternative but still valid emission scenario, it was assumed that 5% of the annual imports during the time of PCB production and import were emitted to the atmosphere. This situation is represented through emissions scenario 2. Constant emissions were taken to be 0.198 tonnes/year which is the average rate of the time-variant emissions of PCB 153 (Scenario 2) from 1930-2100.

Under Scenario 1, emissions peak from 1975-1978 which yields a broader time profile than Scenario 2 (See Supplementary Material, Figure 2). Regardless of this change in profile shape, lifetime exposure is still at a maximum in 1960 and the prenatal and postnatal exposure peaks in 1990 (See Supplementary Material, Figure 2). These maxima correspond to 15 years before and after the maximum in emissions, respectively.



Supplemental Material, Figure 2: Prenatal (dotted line overlapping with dashed line), postnatal (dashed line overlapping with dotted line) and lifetime (solid black lines) exposure time trends relative to emissions (solid gray lines) of PCB 153 under A) scenario 1 and B) scenario 2.

5. Alternate PCB Congeners

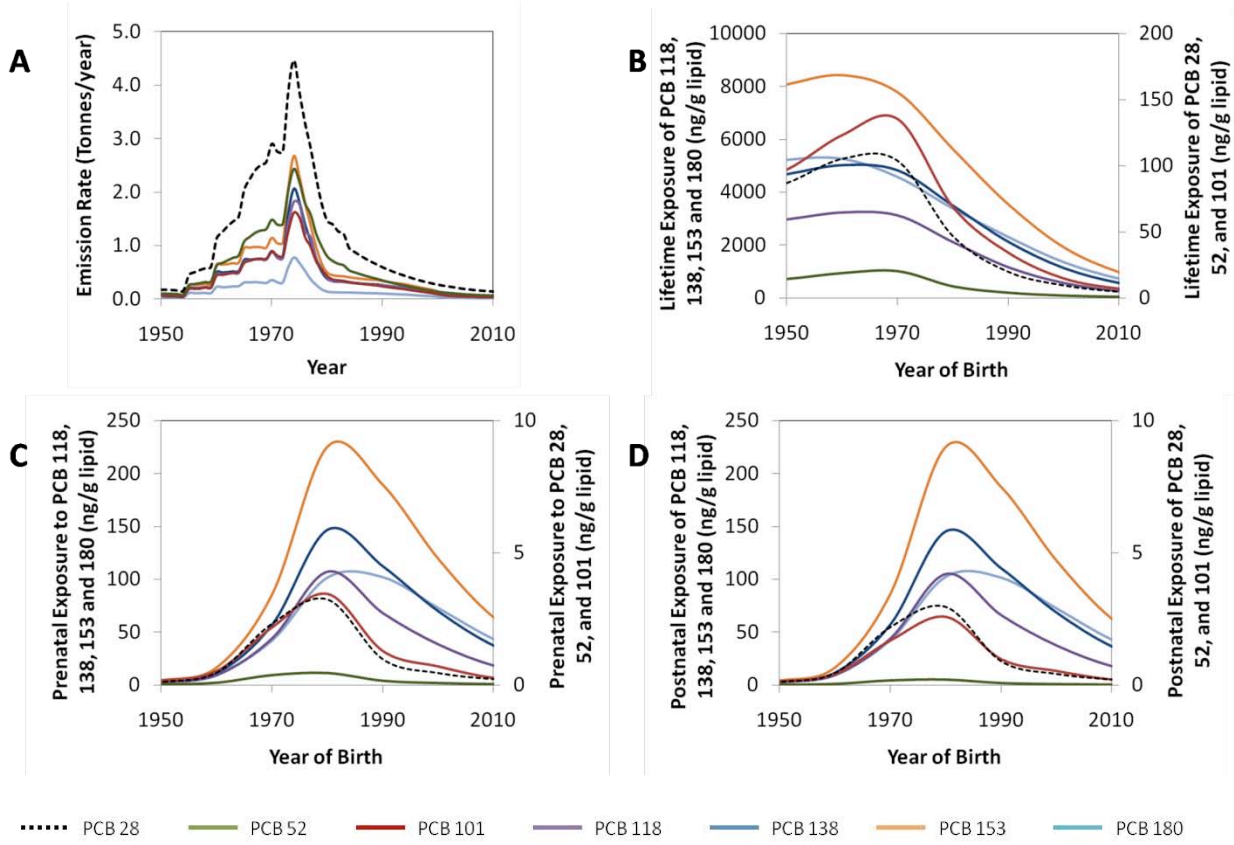
The fates of seven PCB congeners (28, 52, 101, 118, 138, 153, and 180) were modelled according to emissions scenario 2. The physical properties used to model these congeners are outlined in See Supplementary Material, Table 1.

Supplemental Material, Table 1: Partitioning properties of alternate PCB congeners (Breivik et al. 2010)

Chemical	MW (g/mol)	# of Cl atoms	Log K_{OW}	Log K_{OA}	Metabolism Rate Constant (h^{-1})
PCB-28	257.54	3	5.66	7.85	5.48E-5
PCB-52	291.99	4	5.91	8.22	7.42E-4
PCB-101	326.43	5	6.33	8.73	2.28E-5
PCB-118	326.43	5	6.69	9.36	1.26E-5
PCB-138	360.88	6	7.22	9.66	9.13E-6
PCB-153	360.88	6	6.87	9.44	5.25E-6
PCB-180	395.32	7	7.16	10.16	3.42E-7

The IGDE trends predicted for PCB 153 are also applicable to other congeners (See Supplementary Material, Figure 3B-D), however the exact length of the time lag between the peak in prenatal, postnatal, and lifetime exposure relative to the emissions profile decreases with decreasing chlorination (See Supplementary Material, Figure 3B-D). Although the time trends for the different congeners were similar, the extent of bioaccumulation was very different. While the quantity emitted decreased in the order PCB 28, 153, 52, 138, 118, 101, 180 (See Supplementary Material, Figure 3A), the predicted lipid normalized concentration decreased in

the order 153, 138/180, 118, 28/52/101, with cumulative lifetime exposures to PCBs 28,52 and 101 being negligible compared to PCBs 118, 138, 153, and 180 (See Supplementary Material, Figure 3B). These trends largely reflect the impact of the extent of chlorination on the rate of metabolism (Matthews and Dedrick, 1984) and indicate that the parameters dependent upon partitioning behaviour are of relatively minor importance.



Supplemental Material, Figure 3: Time trends A) emissions; B) lifetime exposure; C) prenatal exposure; and D) postnatal exposure of PCB 28, 52), 101,118, 138, 153, and 180.

5. Summary of Simulated Reproductive Characteristics

Supplemental Material, Table 2: Reference Chart for modelled reproductive characteristics of infant and mother under constant and time-variant emission scenarios.

Emissions Scenario	Parameter being modelled	Infant Variable	Maternal Variable	Figure
Constant	# of children	1st born	no children	4A
		2nd born	2 children	
		5th born	5 children	
	maternal age at birth	20, 30, 40	20, 30, 40	4B
	breastfeeding behaviour	breastfed (BM)	breastfeeding (BF)	4C
		Formula fed (FM)	Non-breastfeeding (NBF)	
		healthy	healthy	
Time-variant	# of children	1st born	no children	5A
		2nd born	1 child	
		3rd born	2 children	
		4th born	3 children	
		5th born	4 children	
			5 children	
	maternal age at birth	20, 30, 40	20, 30, 40	5B
	breastfeeding behaviour	breastfed (BM)	breastfeeding (BF)	5C
		Formula fed (FM)	Non-breastfeeding (NBF)	
		healthy	healthy	

References

Breivik K, Sweetman A, Pacyna JM, and Jones KC. 2002. Towards a global historical emission inventory for selected PCB congeners - A mass balance approach: 2. Emissions. Science of the Total Environment 290: 199-224.

Breivik K, Sweetman A, Pacyna, JM, and Jones, KC. 2007. Towards a global historical emission inventory for selected PCB congeners - A mass balance approach. 3. An update. Science of the Total Environment 377: 296-307.

Breivik K, Czub G, McLachlan MS, and Wania F. 2010. Towards an understanding of the link between environmental emissions and human body burdens of PCBs using CoZMoMAN. Environment International 36: 85-91.

Czub G, and McLachlan MS. 2004. A food chain model to predict the levels of lipophilic organic contaminants in humans. Environmental Toxicology and Chemistry 23: 2356-2366.

Matthews HB, and Dedrick RL. 1984. Pharmacokinetics of PCBs. Annual Review of Pharmacology and Toxicology 24: 85-103.

Moser GA, and McLachlan MS. 2002. Modeling digestive tract absorption and desorption of lipophilic organic contaminants in humans. Environmental Science and Technology 36: 3318-3325.

von Goetz N, Wormuth M, Scheringer M, and Hungerbühler K. 2010. Bisphenol A: How the most relevant exposure sources contribute to total consumer exposure. Risk Analysis 30: 473-487.